Computational Science

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SIAM Science Policy Committee

Networking and Information Technology Research and Development Program

- Networking and Information Technology R&D Program (NITRD) helps focus interagency IT R&D:
  - Identify common research needs
  - Plan multi-agency research programs
  - Coordinate and collaborate on research announcements and funding
  - Review research results and adjust accordingly
- Includes R&D programs of twelve participating agencies totaling $2B
- Evolved from the Federal High Performance Computing and Communications Initiative (HPCC), Computing Information and Communications Program (CIC), and Next Generation Internet Program (NGI)
- Assessed by the President's Information Technology Advisory Committee (PITAC)

President's Information Technology Advisory Committee (PITAC)

- **Presidential Advisory IT Committee**
  - Members appointed directly by the President
- **PITAC chartered by Congress in the High-Performance Computing Act of 1991 (P.L. 102-194) and Next Generation Internet Act of 1998 (P.L. 105-305)**
  - The Advisory Committee shall provide the Director [of OSTP] with an independent assessment of:
    - Progress made in implementing the Program
    - The need to revise the Program
    - The balance between the components of the Program
    - Whether the research and development undertaken pursuant to the Program is helping to maintain United States leadership in computing technology
    - Other issues identified by the Director
- **PITAC recommendations have helped guide the NITRD program and its predecessors. Reports available at**
  - http://www.itrd.gov/pitac/

PITAC Computational Science Subcommittee

- Requested by Director of OSTP on June 9, 2004
- Charge letter available at http://www.itrd.gov/pitac/20040609_compsci_charge.pdf
- Charge includes study of
  - Appropriateness of agency research priorities
  - Balance between short and long term research
  - Development vs. application of Computational Science
  - Integration of Computational science training and research into scientific disciplines that apply CS
  - Coordination among agencies
  - Response of agencies to change
  - Elimination or mitigation of barriers to potential of CS
- Subcommittee led by Prof. Dan Reed
- SIAM input very welcome

Context for Request that PITAC Examine Computational Science?

- **Historical Government role in fostering CS**
- **Importance of CS to agency missions**
- **Contribution of CS to economic prosperity**
- **Sense that "all is not well"**
  - Ageing population of computational scientists
  - Difficulty of using current computational environments
  - Limited progress on recognized CS problems (e.g. Lax Report)
  - Concern that CS will not achieve potential
  - Debates about Federal investment strategy (e.g. software maintenance)
- **HECRTF debated many of these issues**
  - see http://www.itrd.gov/hecrtf-outreach/

User and Agency Views on High-End Computing

- **Research pipeline dry**
- **Industrial base issues**
- **Technology improvement demanded by users**
  - **Radical improvements in time-to-solution;**
  - **Better software, algorithms, and ease of use**
  - **Significant improvements to system bandwidth, reliability, ease of programming**
  - **Diversity of architectures**
- **User demand exceeds available resources for both capacity and capability**

PITAC Computational Science Charge

- How well is the Federal Government targeting the right research areas to support and enhance the value of computational science? Are agencies' current priorities appropriate?
- How well is current Federal funding for computational science appropriately balanced between short term, low risk research and longer term, higher risk research? Within these research arenas, which areas have the greatest promise of contributing to breakthroughs in scientific research and inquiry?
- How well is current Federal funding balanced between fundamental advances in the underlying techniques of computational science versus the application of computational science to scientific and engineering domains? Which areas have the greatest promise of contributing to breakthroughs in scientific research and inquiry?

PITAC Computational Science Charge

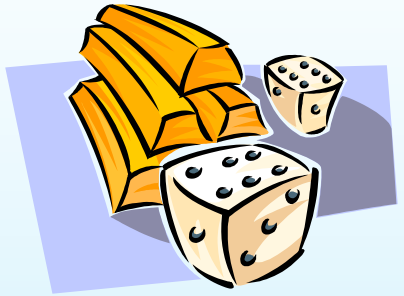
- How well are computational science training and research integrated with the scientific disciplines that are heavily dependent upon them to enhance scientific discovery? How should the integration of research and training among computer science, mathematical science, and the biological and physical sciences best be achieved to assure the effective use of computational science methods and tools?
- How effectively do Federal agencies coordinate their support for computational science and its applications in order to maintain a balanced and comprehensive research and training portfolio?
- How well have Federal investments in computational science kept up with changes in the underlying computing environments and the ways in which research is conducted? Examples of these changes might include changes in computer architecture, the advent of distributed computing, the linking of data with simulation, and remote access to experimental facilities.
- What barriers hinder realizing the highest potential of computational science and how might these be eliminated or mitigated?

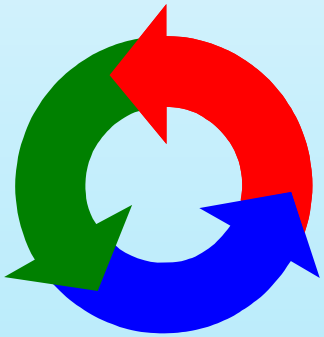
Recent Workshops and Reports

- **Blueprint for Future Science Middleware and Grid Research and Infrastructure, August 2002**
  - http://www.nsf-middleware.org/MAGIC/default.htm
- **NSF Cyberinfrastructure Report, January 2003**
  - http://www.cise.nsf.gov/evnt/reports/toc.htm
- **DOE Science Network Meeting, June 2003**
  - http://gate.hep.anl.gov/may/ScienceNetworkingWorkshop/
- **DOE Science Computing Conference, June 2003**
  - http://www.doe-sci-comp.info
- **DOE Science Case for Large Scale Simulation, June 2003**
  - www.pnl.gov/scales/
- **DOE ASCR Strategic Planning Workshop, July 2003**
  - http://www.fp-mcs.anl.gov/ascr-july03spw
- **High End Computing Revitalization Task Force, 2003-2004**
  - http://www.itrd.gov/hecrtf-outreach/

HECRTF Workshop Recommendations

- **Sustained investment**
  - research, development and system acquisition
    - key to long-term planning and strategic decisions
  - *see the virtuous cycle below*
- **Basic university research**
  - pipeline of ideas and people
    - attracting students and educating a new generation
  - research pipeline sustenance via stable funding
- **Deep collaboration**
  - academic researchers and government laboratories
  - industrial laboratories and computer vendors
  - *lower the barriers for collaboration/technology transfer*
- **Multiple iterations of the virtuous cycle**
  - advanced research and development
  - large-scale system prototyping
  - product development and assessment
  - *deploy, learn, deploy, learn, deploy …*





Upcoming Public Input Opportunities

- **SC04 Birds of a Feather (BOF)**
  - November 10, 5:30-7:00pm, Room 303/304/305
  - National Priorities for Computational Science: A PITAC Town Hall Meeting
  - *3 minute position statements*
  - *Written statements also welcome*

- **Upcoming public PITAC meetings**

For Further Information

Please contact us at:

nco@nitrd.gov

Or visit us on the Web:

www.nitrd.gov

Backup

Agencies and Departments Participating in NITRD Program

- Department of Defense
  - Defense Advanced Research Projects Agency (DARPA)
  - National Security Agency (NSA)
  - Office of the Director of Defense Research and Engineering (ODDR&E)
  - Defense Information Systems Agency (DISA)
- Department of Energy
  - Office of Science (DOE/SC)
  - National Nuclear Security Administration (DOE/NNSA)
- Department of Health and Human Services
  - National Institutes of Health (NIH)
  - Agency for Health Research and Quality (AHRQ)
- Department of Commerce
  - National Institute of Standards and Technology (NIST)
  - National Oceanic and Atmospheric Administration (NOAA)
- National Science Foundation (NSF)
- National Aeronautics and Space Administration (NASA)
- Environmental Protection Agency (EPA)
- Observers: Federal Aviation Administration (FAA), Food and Drug Administration (FDA)